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PREDICTION OF DROPLET TEAR-OFF AND MENISCUS FORMATION IN THE TOP-SPOT EXPERIMENT USING TRANSAT

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ABSTRACT

For the design and development of new microfluidic devices reliable modeling and simulation tools must be made available. Many extensions to conventional computational fluid dynamics are required, especially multiphase fluid dynamics simulation capability. A new dynamic contact angle model is presented here, which does not require the specification of a contact angle or contact–line velocity. The level-set method is used for interface capture. The model is tested for unit problems such as relaxation to equilibrium of a contact line. It is then applied to the problem of fluid filling in a prototypical microdevice to show its utility as a design tool.

INTRODUCTION

Microfluidic devices are now used for such diverse applications as DNA microarrays, drug screening, sensors, and in clinical and forensic analysis. Typical microfluidics flows feature free-surface motion evolving (sometimes) in porous media or as falling films, spreading and dewetting of (complex) liquids on solid or liquid substrates, chemical reaction of binary mixtures, micro-bubbles and beads control and manipulation, phase change or transition. The control of such micro-flow systems is central to future technological advances in emerging technologies, like biological reactors, microreactors, biochannel arrays, and labs-on-chip [6]. It is expected that robust, accurate and fast response computational microfluidics solutions will play a key role in the development in this new business segment. In practical applications the flow involves phenomena acting at different time and length scales. At each level of the scale cascade, the physics of the flow is amenable to numerical prediction by scale-specific strategies. Microfluidic technologies have developed rapidly over the past few years. However, mature design support, in terms of modeling and simulation tools is yet largely unavailable. In particular, many extensions to conventional computational fluid dynamics (CFD) are required: small scale physical effects such as surface forces, dynamics of three–phase contact lines, heterogeneous chemical reactions, surfactants, etc. are some obvious examples.

Incompressible two-phase flows with moving contact lines are common in a variety of applications, such as coating and biological processes. One of the difficulties in simulating such flows is that the Navier-Stokes equations for both fluids, in combination with no-slip boundary conditions, predict a shear stress singularity at the contact line. Also, the contact angle made by the interface with the solid surface needs to be specified. Several attempts have been made in the past decades to model contact–line dynamics within the continuum fluid dynamics framework. Generally, models are used where contact angles are prescribed based on front velocities and criteria for advancing and receding scenarios [1]. However, these models do not take into account the physical forces acting in the triple line region. The model presented in this study is based on the molecular dynamics [2] description of the contact–line, such that it does not require the specification of contact angles. Instead of specifying the contact angle a force is added to the momentum equations which is based on the Young's law and is referred to as the unbalanced

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Young force [3]. The stress singularity at the contact line is regularized using a slip length and integrating the logarithmic singularity upto the slip length. The model is validated and compared to unit simulations presented by Spelt [1]. The computational model could in some cases be used in conjunction with a sub-grid scale (SGS) ultra-thin film model for similar microfluidics flows (more in biological systems), though involving separate droplet motion in wet tubes to avoid numerical dry-out, or liquid film breakup at the contact with the wall. Another experiment is also simulated to validate this SGS model. The coupled approach is used here in 2D axisymmetric conditions to analyze droplet tear-off and meniscus formation in the TopSpot experiment [7].

SIMULATION FRAMEWORK

The Microfluidics code TransAT [4] is a multi-physics, finite-volume code based on solving multi-fluid Navier-Stokes equations on structured multi-block meshes. MPI parallel based algorithm is used in connection with multi-blocking. Grid arrangement is collocated and can thus handle more easily curvilinear skewed grids. The solver is pressure based, corrected using the Karki-Patankar technique for weak compressible flows. The Navier-Stokes and level set equations are solved using the 3rd order Runge-Kutta explicit scheme for time integration. The convective fluxes are discretized with TVD-bounded high-order schemes. The diffusive fluxes are differenced using a second order central scheme. Multiphase flows are tackled using both the phase-average homogeneous model for macro-scale multiphase flows and the one-fluid formulation for interfacial microfluidics flows. The one-fluid formulation on which TransAT is built is such that a two–fluid flow is viewed as a single fluid having material properties varying according to a colour function which distinguishes the boundary or interface between the two fluids. Specifically, both the Level-Set, Phase Field and the Volume-Of-Fluid (VOF) Interface Tracking Methods (ITM) can be employed to track evolving interfaces. TransAT deals with phase change, surface tension and triple-line dynamics, Marangoni effects, and micro-film sub-grid scale modeling for lubrication.

Interface Tracking Methods (ITM)

When the exact shape of the interfaces separating two fluids is not known, or not relevant, one may resort to the averaged Two-Fluid approach, where separate conservation equations are required for each phase with appropriate interfacial exchange forces. ITMs are invoked when the identification of interfaces needs to be precise, as in the breakup of large bubbles, droplets or liquid jets. The key to these methods is the use of a single-fluid set of conservation equations with variable material properties and surface forces. The concept is attractive, since it offers the prospect of a more subtle strategy than that offered by the two-fluid formalism, while minimizing modeling assumptions.

Transport Equations

The incompressible fluid dynamics equations expressed within the single-fluid formalism take the following form,

$$\frac{\partial \rho}{\partial t} + u_j \frac{\partial \rho}{\partial x_j} = 0 \tag{1}$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} - \frac{\partial \sigma_{ij}}{\partial x_j} = b_i + s_i + c_i \tag{2}$$

where the RHS terms in the momentum equation (Eq. 2) represent the body forces, the surface tension expressed by Eq. 4 below, and its contact–line wall contribution, respectively. In Eqs. (1-2), where phase change could be accounted for, σ_{ij} is the Cauchy stress tensor, representing pressure and viscous forces.

In the level-set method [9] the interface between two fluids is represented by a continuous function ϕ, representing the distance to the interface that is positive on one side and negative on the other. This way, both fluids are identified, and the location of the physical interface is associated with the zero level. The level-set evolution equation is given by

$$\frac{\partial \phi}{\partial t} + u_j \frac{\partial \phi}{\partial x_j} = \dot{m}/\rho |\nabla \phi| \tag{3}$$

In the above equation $\dot{m}$ stands for the heat/mass transfer rate [8], which can be either directly determined using the energy jump across the interface, or modeled using heat transfer correlations. Material properties are updated locally based on ϕ and smoothed across the interface using a modified Heaviside function. Further, the fact that ϕ is a continuous function across the interface helps determine the normal vector n_i to the interface, and thereby the surface curvature required for the definition of the surface tension,

$$s_i = \gamma \kappa n_i \delta^I(\phi) + \nabla_s(\gamma)\delta^I(\phi) \tag{4}$$

where γ is the surface tension of the fluid pair, *kappa* is the interfacial curvature defined as $\kappa = -\nabla\phi/|\nabla\phi|$, δ^I is a smoothed Dirac delta function centered at the interface. The last term in the equation above is introduced to model the Marangoni effects related to the rate of change of the surface tension coefficient due to temperature or surfactant concentration. Material properties (density, the viscosity, heat capacity, thermal conductivity) are updated locally based on ϕ and distributed across the interface using a smooth Heaviside function $H(\phi)$.

The level set function ceases to be a signed distance from the interface after advecting Eq. 3. To restore its correct distribution near the interface, a re-distancing equation is solved:

$$\frac{\partial d}{\partial \tau} - sgn(d_0)(1 - |\nabla d|) = 0 \tag{5}$$

where $sgn(x)$ is the Signum function, and $d_0(\mathbf{x},t) = \phi(\mathbf{x},t)$. In TransAT the above equation is solved after each advection step of Eq. (3) using the non-oscillatory (WENO) 3^{rd} order scheme.

Dynamic Contact Angle Model

The present work proposes a method for the numerical treatment of wetting dynamics based on the physical forces associated with triple lines [5]. A triple line force included in the momentum equation; this extended momentum equation could then provide a physically adequate description of wetting dynamics, eliminating the need for any particular boundary condition specifying the contact angle. The triple line force used in the present work is based on a consideration of interfacial free energy [3]. Accordingly, it contains only two parameters: the interfacial tension between the fluids γ and the equilibrium contact angle θ_{eq}.

$$c_i = \gamma(\cos(\theta_{eq}) - \cos(\theta_{dy}))\delta_t b \tag{6}$$

where θ_{dy} is the instantaneous dynamic contact angle, δ_t is a Dirac delta function vanishing everywhere except on triple lines, with the property that for any volume V, the integral $\int_V \delta_t dV$ is equal to the length of the triple line segment contained in V, and b is the unit vector normal to the triple line and parallel to the wall surface. The triple line force, is obtained by considerations similar to the derivation of Youngs Law and can be referred to as the unbalanced Young force [3].

The second issue to be dealt with for a successful simulation method for contact line dynamics is the resolution of the stress singularity that arises due to the no–slip boundary condition. In the current model, the shear stress is assumed to have a logarithmic profile as it nears the contact line [2]. At distances less than a slip length from the contact line, full slip is assumed. In the finite volume containing the contact line, the integrated shear stress is applied. The slip length is taken to be a small value $\approx 10^{-9}$m.

Subgrid-scale ultra thin-film modeling

In some microfluidics problems involving drop motion, an ultra-thin film flows at the walls and needs to be treated by resorting to detailed multiphysics, interfacial flow simulation. The presence of a singular-point in flows through junctions for example controls the drop dynamics and rupture. In the junction a thin film is formed preventing bubble breakup. This can be predicted only with high-fidelity simulations using a SGS model for thin film, and contact angle treatment for wetting. Without multiscale treatment the models will fail to deliver accurate and physical sound results. The drop will breakup producing a non-physical solution (i.e. numerical dry-out) whereas wetting should sustain) as the drop enters in the junction. Multiscale simulation of thin film flow is necessary here, requiring SGS thin-film models and wetting capabilities. The ultra-thin film SGS model implemented in TransAT for this class of flow is based on a modified model of the Taylor [10] thin-film theory, which originally proposes to model the height of a thin film as a function of the fluid Capillary number $Ca = \mu U/\gamma$; i.e.

$$\frac{\delta}{r} = 1.337Ca^{2/3}, \tag{7}$$

where r stands for the pipe radius, and U for the (characteristics) speed of the bubbles inside the tube. This is found to be valid in the range $10^{-04} < Ca < 1$. Aussillious and Quere [11] revisited the original Taylor's hypothesis (7) and proposed for the visco-capillary deposition regime, the following model:

$$\frac{\delta}{r} = \frac{1.34Ca^{2/3}}{1 + 1.34 * 2.25Ca^{2/3}} \tag{8}$$

which he has shown to fit with the experimental data for $10^{-02} < Ca < 1$. The models are implemented in TransAT.

Numerical Details

The Navier-Stokes transport equations and the level set advection function are solved using the 3rd order Runge-Kutta explicit scheme for time integration of all variables. The convective fluxes are discretised using the 3rd order Quick scheme bounded using a TVD limiter. The diffusive fluxes are differenced using a 2nd order central scheme. In the cases presented in this paper, Marangoni effects and phase change mass transfer do not apply.

MODEL VALIDATION

Relaxation to equilibrium

We consider here two cases presented by Spelt [1] of a droplet that is immersed in a different fluid, and adhering to a long boundary of a rectangular domain (2×1, discretised by $2N \times N$). In Case I, the densities are equal ($= 1$) whereas the viscosities differ (droplet 4.95×10^{-2}, surrounding phase 4.95×10^{-3}). A density contrast is used in Case II (droplet 1 and surrounding fluid 20) however, with constant viscosity 4.95×10^{-2}. The surface tension coefficient was chosen to be $\gamma = 0.11$ and 2.21 for the two cases, respectively and the simulations were performed for a 2D mesh size of $128x64$. To begin with the droplets are circular caps (radius 1.66), with contact angles being 30^o and 150^o for the dark phase (blue in Figs. 1 and 2), which is different from the equilibrium contact angles $\theta_{eq} = 120^o$ and 60^o, respectively. The main difference of the current model from the model of Spelt [1] is that the latter case requires the additional specification of a contact–line velocity. Figures 1 and 2 show the return to equilibrium for Cases I & II, respectively. The variation of the contact angles as the flow evolves to equilibrium

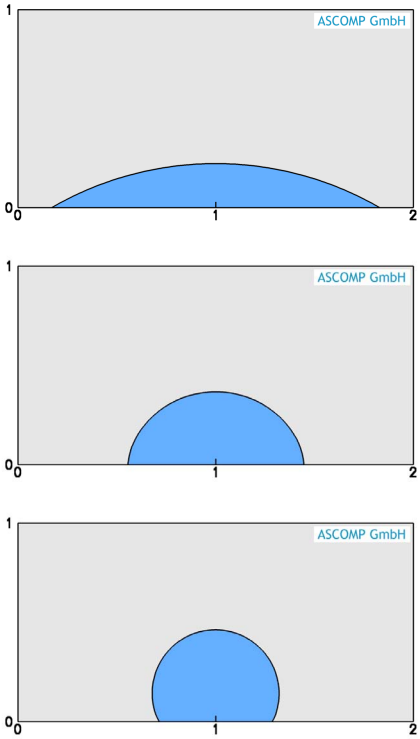

FIGURE 1. RETURN TO EQUILIBRIUM FOR A NON-WETTING LIQUID; $\theta_{eq} = 120^o$, at $t = 0s$, $t = 3.7s$ and $t = 19.8s$. Axes in [mm]

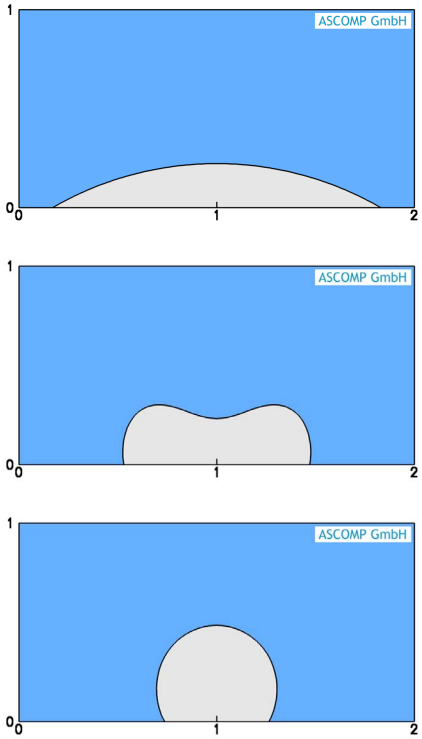

FIGURE 2. RETURN TO EQUILIBRIUM FOR A WETTING LIQUID; $\theta_{eq} = 60^o$, at $t = 0s$, $t = 0.6s$ and $t = 3.6s$. Axes in [mm]

is shown in Fig. 3. In Case II a faster return to equilibrium is seen driven by the higher surface tension along with an overshoot due to the higher density of the outer phase.

Droplet motion in a microchannel

The results depicted in Fig. 4 clearly show that without a thin-film model, numerical dry-out will occur (panel a). Our SGS model is able to take into account the effect of lubrication by imposing a liquid film thickness, thus allowing for a smooth transport of the bubbles at low Capillary number (1mm D channel containing air and water, for $Ca = 0.001546$). The inflow liquid and gas velocities are 0.111 and $0.066 m/s$, respectively.

The Topspot Micro Array Problem

Topspot® is a microarray technology dedicated to generate hundreds of nanoliter droplets at once using an external pressure pulse. The simulation is done as a validation case for the level set implementation in TransAT© and the code itself. The present comparison is based on the paper of Glatzel et al. [7], in which the results of various CFD softwares (Fluent, CFX and CFD-ACE+) were compared (in 3D) to the data. In contrast the model is applied here in 2D axisymmetric, as shown in Fig.

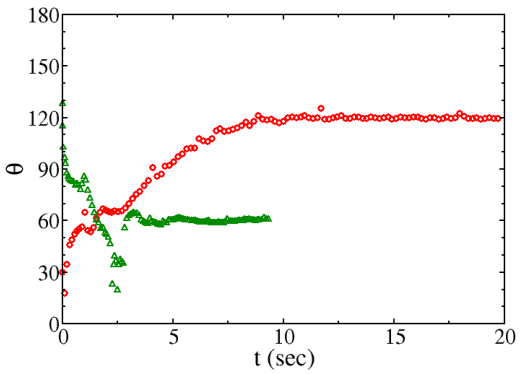

FIGURE 3. VARIATION OF CONTACT ANGLE WITH TIME. Red - Case I; Green - Case II.

(5). The overall domain size is $200\ \mu m \times 880\ \mu m$ and contains 19564 cells, refined to the nozzle whose diameter of $50 \mu m$ is resolved with 20 cells. Therefore the minimum grid spacing is $h = 2.5\ \mu m$. The level set method is used instead of VOF. The walls exposed to the liquid - gas - interface are partial wetting at a static contact angle of 130°. For driving the droplet genera-

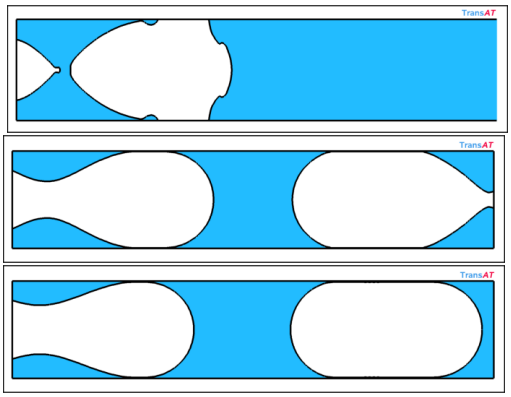

FIGURE 4. SGS THIN-FILM MODEL IN A MICROCHANNEL; $\delta/L = 0; 5 and 10\mu m$. $\delta/r = 0$; $\delta/r = 5\mu m$; $\delta/r = 10\mu m$.

tion a time dependent boundary condition was applied on top of the domain. In this study, two different pressure curves are compared, as presented in Fig. (6). The blue points mark the most significant data of the experimentally measured pressure curve. The data are approximated (red curves) using a sinusoidal and a harmonic pressure-pulse functions, reading respectively:

$$p(x) = 0.175 \cdot \sin\left(\frac{2\,\pi\,t}{800}\right) \tag{9}$$

$$p(x) = 0.13 \cdot \sin\left(\frac{2\pi t}{800}\right) + 0.03 \cdot \sin\left(\frac{2\pi t}{111} + 3.2\right) \tag{10}$$

The harmonic curve is used trying to reproduce the characteristic points of the experimental pressure curve. For the simulation, the implicit scheme is used together with the 4th order Runge-Kutta and the HLPA discretization for the time and the convection, respectively. The non - dimensional numbers are calculated to estimate a first time step for the calculation. Their maximum value is set to be 0.5 and their minimum value to be 0.3. The resulting reference velocity is $u_0 = 0.163\ m/s$. As the energy equation is not solved, the Fourier criterion does not restrict the time step. In the beginning, the interface between the two phases is flat, so that also the surface tension criterion does not dictate the time stepping. The CFL number results in a time step of $\Delta t = 7.6e-6\ s$ and the diffusion number yields $\Delta t = 1.56e-6\ s$. The diffusion restricts the time step most, but it is not the governing process in the simulation. Therefore, the maximum is set to higher values in order to let the CFL number restrict the time step. The simulation began with a time step of $\Delta t = 1e-7\ s$ as the calculated velocity is only an estimation but using the time step adaptation abilities of TransAT©.

This fully transient problem is solved by the TransAT© code within 3:22:30 hours using an adaptive time step of approximately 5 μs. The results using the two pressure boundary conditions compared with the experiments according to Glatzel et

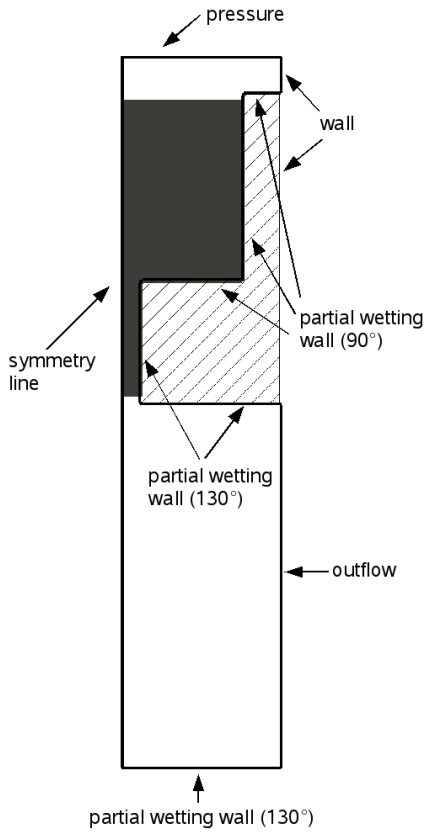

FIGURE 5. Topspot® - DOMAIN AND BOUNDARIES

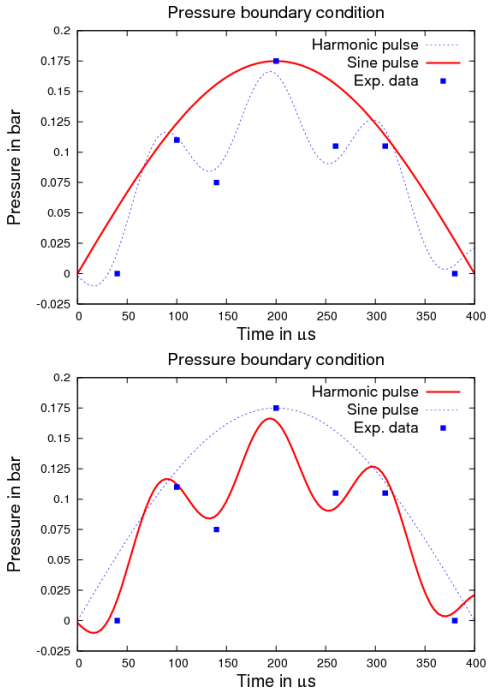

FIGURE 6. MODELLED PRESSURE CURVES.

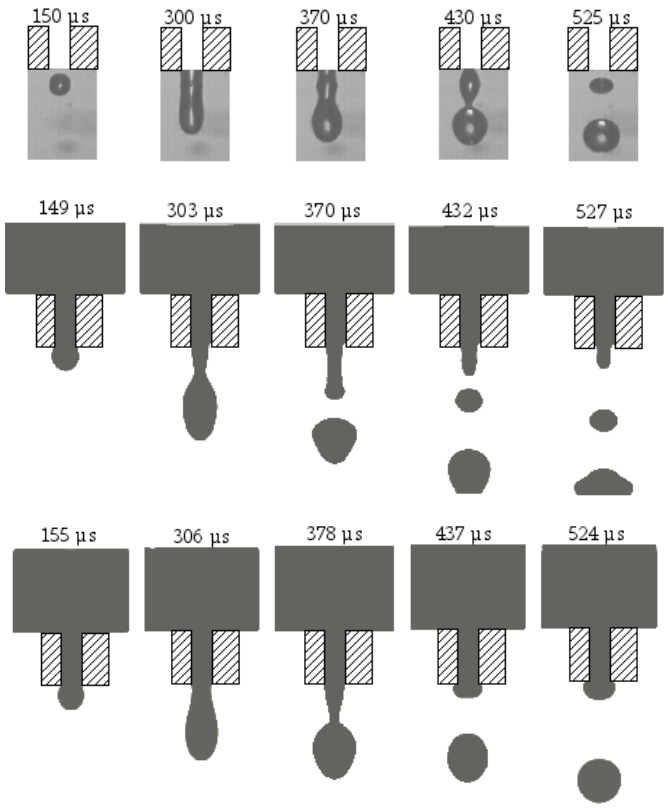

FIGURE 7. COMPARISON OF TransAT WITH THE DATA (top= Exp.; middle= sine pulse; bottom=harmonic pulse.

al. [7] are presented in Fig. (7). Using only a sine pressure curve is not sufficient to produce the same droplet characteristics as given in the experimental data. The tear-off time is already at 339 μs what is too early compared with the experimental value being at about 450 μs. In addition, a satellite drop is produced enlarging the volume of the dispersed fluid shown for 432 μs in Fig.(7 b). Fig.(7 c) presents the results for the harmonic pressure pulse preserving a satellite drop. The tear-off time of 394 μs is also better compared to the former results. The droplet volume of 0.9 *nl* is larger than in the experiment being 0.68 *nl* but the value is in the range of the two successfully tested CFD codes in the above mentioned paper [7] presenting 0.66 *nl* for CFD-ACE+ and 1.4 *nl* for CFX. It has to be pointed out that compared to the tested codes only TransAT© is capable to predict a droplet remaining attached to the nozzle after the tear-off.

Summary

A new dynamic contact angle model has been presented for the simulation of microfluidic flows. The model uses a force in the momentum equation instead of specifying the contact angle or a contact–line velocity. The model could be used in conjunction with a sub-grid scale ultra-thin film model for similar microfluidics flows involving separate droplet motion in wet tubes. The model implementation in TransAT was tested for the TopSpot droplet generator problem which involves precise droplet breakup dynamics. It was clearly observed that the droplet tearoff is strongly affected by the imposed pressure forcing and a precise control is required to obtain specific break up. The results obtained using TransAT compare very well to the data; better than those obtained using other softwares [7].

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